



Truchas Flow Models

Truchas Workshop January 22-23, 2003

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Flow Model Requirements

- Time-accurate solution of the Navier-Stokes equations
- Multiple Materials (with widely varying densities)
- Complex three dimensional geometry // *multiple size scales*
- Varied boundary and initial conditions
- *Verification and Validation*
- Transient interface tracking
- Normal and tangential surface tension forces
- Transport of enthalpy and species
- Turbulent diffusion of momentum, *enthalpy, species*
- Buoyant flow (temperature, species)
- Mushy zone flow
- *Significant density changes*
- Coupling to thermal state // *stress distortion*

Mesh Geometry and Variables

- *Three dimensional (x, y, z) coordinates*
- *Internal orthogonal mesh generator*
- *Non-orthogonal mesh reader (multi formats)*
 - *Hexahedra, prisms, tetrahedra*
- *Co-located, cell-centered variables*
 - *Face velocities for fluxing*
- *Automatic Mesh Partitioning for 2 level preconditioning (Chaco)*
- *"Monte Carlo" initialization of material bodies*



Flow solution within the overall time step advancement

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- *Flow starts each cycle*
 - Preliminary step on first cycle (solenoidal velocity)
- *Flow may limit time step size*
- *Enthalpy advection added at the start of the enthalpy solution*
- *Solidification also changes material and species concentrations*



Continuum Equations

$$\frac{\partial}{\partial t}(\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \vec{u}) = \vec{F}_S + \vec{F}_D + \vec{F}_L + \rho' \vec{g} + \nabla \cdot \vec{\tau}$$

$$\nabla \cdot \vec{u} = 0 \quad \vec{\tau} = \mu_t \nabla \vec{u} - P \vec{I}$$

$$\frac{\partial \rho}{\partial t} + \vec{u} \cdot \nabla \rho = 0$$

$$\vec{F}_D = -\vec{c}_d \cdot \vec{u} \quad \vec{c}_d = \frac{(1-f^2)}{f^3} \vec{I} \cdot \vec{C}_p$$

Fractional-Step Solution Order

- *Interface reconstruction and volume tracking*
 - *Advect momentum, enthalpy, species*
- *Partially implicit velocity prediction*
- *Transfer to face (fluxing) velocities*
 - *Rhie-Chow procedure*
- *Cell-centered projection solution*
 - *Solenoidal fluxing velocity field*
- *Correct cell-centered velocity vector*

Volume Tracking Formalism

$$\frac{\partial f_k}{\partial t} + \mathbf{u} \cdot \nabla f_k = 0 \quad \Rightarrow \quad \frac{\partial f_k}{\partial t} + \nabla \cdot (\mathbf{u} f_k) = f_k \nabla \cdot \mathbf{u}$$

$$V_k = \int f_k dV$$

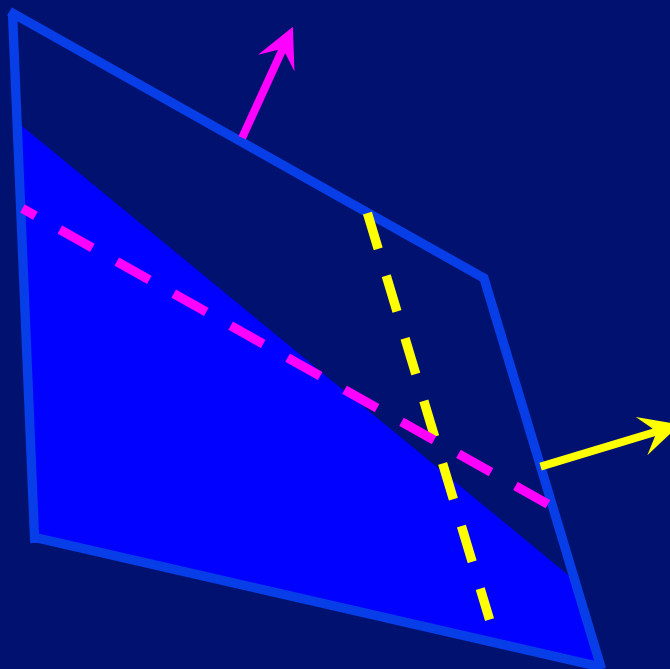
$$\frac{\partial V_k}{\partial t} + \int \nabla \cdot (\mathbf{u} f_k) dV = \int f_k (\nabla \cdot \mathbf{u}) dV$$

$$V_k^{n+1} - V_k^n + \sum_f \delta V_{k,f}^n = 0$$

Piecewise Linear Reconstruction

➤ *Construct planar interfaces within each cell*

- *Normal estimated by Green-Gauss*



- *sub cycling*

Predictor Step for the Cell-Centered Velocity

$$\rho_c^{n+1} \vec{u}_c^* = \rho_c^n \vec{u}_c^n + \delta t \left[\rho_c^{n+1} \vec{u}_f^n \cdot \nabla \vec{u}_c^n - \rho_c^{n+1} \left\langle \frac{\nabla P^n}{\rho_f^n} - \frac{\rho_f^n + \delta \rho_f^n}{\rho_f^n} \vec{g} \right\rangle_c + \nabla \cdot \vec{\tau}_t + \vec{F}_D \right]$$

$$\vec{F}_D = -\vec{c}_d \cdot \vec{u}^*$$

$$\nabla \cdot \vec{\tau}_t = \nabla \cdot \mu_t^{n+1} \nabla \left(\theta \vec{u}^* + (1 - \theta) \vec{u}^n \right)$$

➤ *Solve using linear solver as necessary*

Transfer cell-centered velocity to face centroids ¹⁰

- Use a Rhie-Chow like approach
 - Pressure gradient and Boussinesq force

$$\vec{u}_c^* + \delta t \left\langle \frac{\nabla P^n}{\rho_f^n} - \frac{\rho_f^n + \delta \rho_f^n}{\rho_f^n} \vec{g} \right\rangle_c \xrightarrow{\text{transfer}} \vec{u}_f^\dagger$$

$$\vec{u}_f^* = \vec{u}_f^\dagger - \delta t \left[\frac{\nabla P^n}{\rho_f^{n+1}} - \frac{\rho_f^n + \delta \rho_f^n}{\rho_f^{n+1}} \vec{g} \right]_f$$

Cell-centered projection step

- *Project the face velocities onto a Solenoidal field*
- *Solve for the change in pressure*

$$\begin{aligned}\vec{u}_f^{n+1} &= \vec{u}_f^* - \delta t \left[\frac{\nabla \delta P^{n+1}}{\rho_f^{n+1}} - \left(\frac{\rho_f^{n+1} + \delta \rho_f^{n+1}}{\rho_f^{n+1}} - \frac{\rho_f^n + \delta \rho_f^n}{\rho_f^{n+1}} \right) \vec{g} \right]_f \\ &= \vec{u}_f^* + \delta t \left(\frac{\rho_f^{n+1} + \delta \rho_f^{n+1}}{\rho_f^{n+1}} - \frac{\rho_f^n + \delta \rho_f^n}{\rho_f^{n+1}} \right)_f \vec{g} - \delta t \frac{\nabla \delta P^{n+1}}{\rho_f^{n+1}} \Big|_f\end{aligned}$$



Cell-centered velocity correction

- *Update for the modified pressure and Boussinesq force*
- *Average these terms over all cell faces*

$$\frac{\vec{u}_c^{n+1} - \vec{u}_c^*}{\delta t} = - \left\langle \frac{\nabla \delta P^{n+1}}{\rho_f^{n+1}} - \left(\frac{\rho_f^{n+1} + \delta \rho_f^{n+1}}{\rho_f^{n+1}} - \frac{\rho_f^n + \delta \rho_f^n}{\rho_f^{n+1}} \right) \vec{g} \right\rangle_c$$



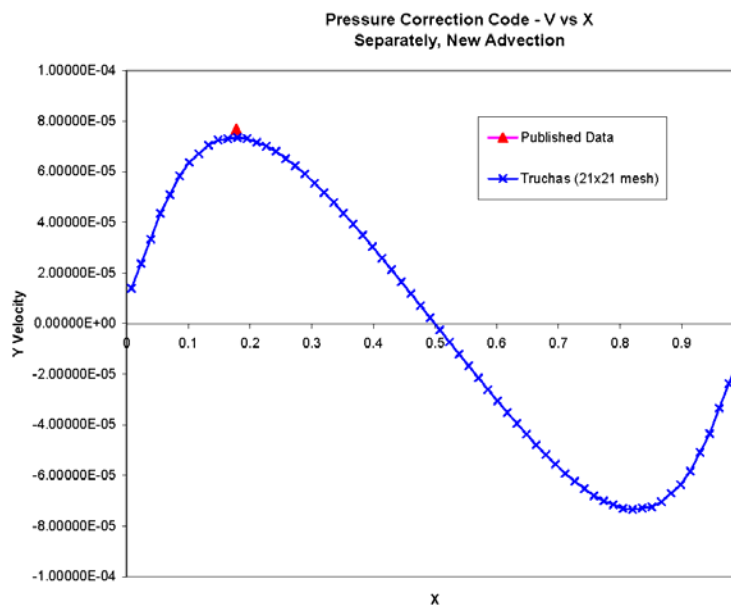
Verification / Validation

- *Poiseuille flow in ducts and pipes*
- *Backward facing step (low Re)*
- *de Vahl Davis natural convection benchmark*
- *Lid driven cavity benchmark (Ghia)*
- *Voller-Prakash solidifying flow*
- *Porous media pressure drop*
- *Baneczek freezing test*
- *SCN solidification Benchmark*

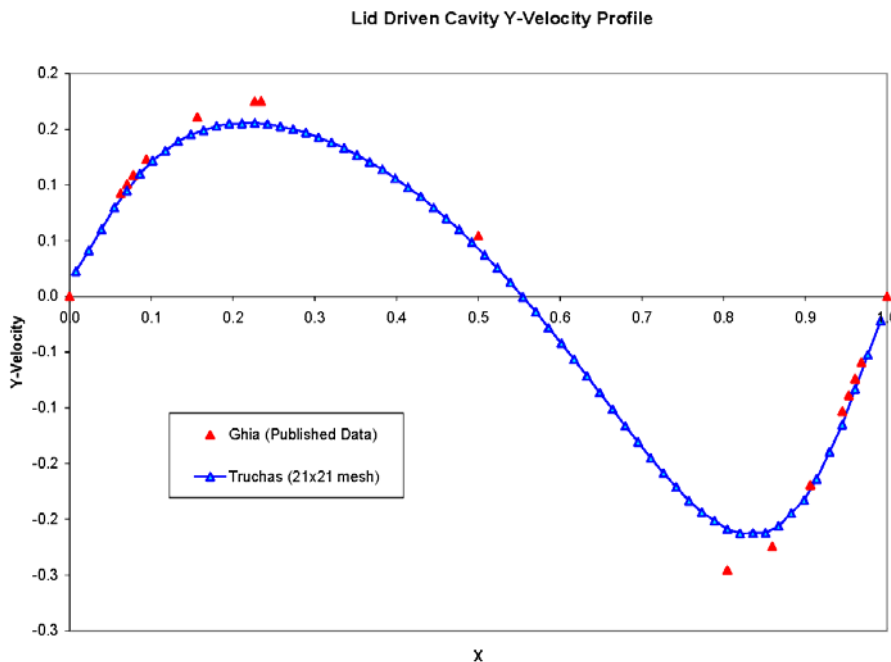
(Thanks to Jeff Marchetta for many of these calculations.)

de Vahl Davis benchmark vertical velocity comparison

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Lid driven cavity horizontal velocity comparison



Future Directions

- *Modeling flow in the mushy zone*
- *Higher order spatial operators*
- *Local Runge-Kutta*
- *Reduced computing cost*
- *Turbulence model improvements*
- *Immersed boundary method*
- *Improved interface tracking*